Striped phases in the two-dimensional Hubbard model with long-range Coulomb interaction

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We investigate the formation of partially filled domain walls in the two-dimensional Hubbard model in the presence of long-range interaction. Using an unrestricted Gutzwiller variational approach we show that: i) the strong local interaction favors charge segregation in stripe domain walls; ii) The long-range interaction favors the formation of half-filled vertical stripes with a period doubling due to the charge and a period quadrupling due to the spins along the wall. Our results show that, besides the underlying lattice structure, also the electronic interactions can contribute to determine the different domain wall textures in Nd doped copper oxides and nickel oxides.

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The occurence of charged domain walls in the high-T_c superconductors presently attracts a lot of interest also with regard to possible pairing scenarios [1–3]. Incommensurate spin correlations have first been observed in $La_{2-x}Sr_xCuO_4$ (LSCO) by neutron scattering experiments [4–6]. More recently it was found that the incommensurate spin fluctuations are pinned in Nd doped LSCO and nickel oxide compounds [7–9] leading to spin- and charge-stripe order in these materials [10]. However, whereas the domain walls in the hole-doped La_2NiO_4 system are oriented along the diagonals of the NiO_2 lattice, it turns out that in $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$ the orientation of the stripes is along the Cu-O bond direction. Moreover, the hole concentration in the domain walls is one hole per Ni site in the nickelates and one hole every second Cu site in the Nd-doped cuprates. A comparison of the low-temperature orthorhombic and the low-temperature tetragonal structure suggests that the vertical stripes in $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$ are pinned by the tetragonal lattice potential whereas the orthorombic phase in the nickel oxides favors a diagonal orientation. We will show here that the electronic interactions may also play an important role in establishing different domain wall structures.

The stripe instability for doped antiferromagnets was predicted theoretically in [11] within Hartree-Fock (HF) theory applied to the extended Hubbard model and confirmed by a number of subsequent investigations [12]. For small values of the Hubbard on-site repulsion U (generally smaller than $3t$ - $4t$) these calculations result in a striped phase oriented along the (10)- or (01)-direction whereas for higher values of U the orientation is along the diagonals. Within HF theory the stripe solutions become unstable for $U > 8t$ towards the formation of isolated spin-polarons.

However, all stripe calculations performed so far within the HF approximation of the Hubbard model predict one hole per site along the domain wall (filled stripe) [13]. This contrasts the observation of half-filled stripes (i.e. with half a hole per site) in the $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ system which is a yet unresolved problem of mean-field theory. In Ref. [14] it was addressed the question whether the inclusion of an additional nearest neighbor repulsion V in the Hubbard-hamiltonian may favor the formation of partially filled stripes. According to Ref. [14] the half-filled stripe solution is stabilized by a quadrupling of the charge- or spin-period along the stripe. However, although the nearest neighbor repulsion slightly enhances the stability of the half-filled wall this never corresponds to the HF ground state for realistic parameter values. Instead the main effect of V is to shift the crossover to isolated spin polarons to lower values of U.

In the present paper we show that a proper treatment of the strong local repulsion U plays an indirect but crucial role in stabilizing half-filled vertical domain walls. Specifically we apply a slave-boson version of the Gutzwiller approach within an unrestricted variational scheme. Contrary to the pure HF approach, which heavily underestimates the effective attraction between the charge carriers and predicts repulsion for $U > 6t$, it was recently shown that within the slave-boson scheme the attraction persists up to very large U [15]. As a consequence of this more suitable treatment of the strong coupling limit, U greatly favors the charge segregation in striped domains as opposed to spin polarons. In the absence of long-range (LR) forces, completely filled diagonal stripes stay more stable than half-filled vertical ones. However, due to their increased stability with respect to isolated polarons, the stripe solutions now allow for a less disruptive introduction of stronger LR forces, which affect the completely filled stripes more than the half-filled ones. Then, for a sizable but still realistic LR repulsion, the half-filled vertical stripe may become the ground-state configuration.

We consider the two-dimensional Hubbard model on a square lattice, with hopping restricted to nearest neigh-

bors (indicated by the bracket $< i, j >$) and an additional LR interaction:

$$H = -t \sum_{<ij>,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \sum_{i \neq j,\sigma\sigma'} V_{ij} n_{i,\sigma} n_{j,\sigma'} \tag{1}$$

where $c_{i,\sigma}$ destroys an electron with spin σ at site i, and $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$. U is the on-site Hubbard repulsion and t the transfer parameter. For all calculations we take $t = 1$. For the Coulomb potential we assume an interaction of the form $V_{ij} = \frac{V_0}{\sqrt{(\mathbf{R_i}-\mathbf{R_j})^2+\alpha^2}}$ where the parameters V_0 and α are specified through the on-site repulsion U and the nearest-neighbor interaction $V_{n,n+1}$ via $\alpha = V_{n,n+1}/\sqrt{U^2 - V^2_{n,n+1}}$ and $V_0 = \alpha U/2$. Since we consider a finite lattice with periodic boundary conditions it is also necessary to restrict the LR part to half of the lattice dimension both in x- and y-direction.

Following Kotliar and Ruckenstein [16] we enlarge the original Hilbert space by introducing four subsidiary boson fields e_i, $s_{i,\uparrow}$, $s_{i,\downarrow}$, and d_i for each site i. These operators stand for the annihilation of empty, singly occupied states with spin up or down, and doubly occupied sites, respectively. Since there are only four possible states per site, these boson projection operators must satisfy the completeness constraints $e^\dagger_i e_i + \sum_\sigma s^\dagger_{i,\sigma} s_{i,\sigma} + d^\dagger_i d_i = 1$ and $n_{i,\sigma} = s^\dagger_{i,\sigma} s_{i,\sigma} + d^\dagger_i d_i$. In the saddle-point approximation, all bosonic operators are treated as numbers. Furthermore we will approximate the LR part by a HF decoupling. The resulting effective one-particle Hamiltonian describes the dynamics of particles where the hopping amplitude between states (i,σ) and (j,σ) is renormalized by a factor $z^\dagger_{i,\sigma} z_{j,\sigma}$ with $z_{i,\sigma} = \left(e^2_i + s^2_{i,-\sigma}\right)^{-1/2} \left(e_i s_{i,\sigma} + s_{i,-\sigma} d_i\right) \left(d^2_i + s^2_{i,\sigma}\right)^{-1/2}$ The effective one-particle Hamiltonian can be diagonalized by the transformation $c_{i,\sigma} = \sum_k \Phi_{i,\sigma}(k) a_k$ where the fermion wave functions $\Phi_{i,\sigma}(k)$ obey the orthonormality constraint $\sum_{i,\sigma} \Phi^*_{i,\sigma}(k) \Phi_{i,\sigma}(q) = \delta_{kq}$.

Given a system with N_{el} particles we obtain for the total energy

$$E_{tot} = -t \sum_{<ij>,\sigma} z^*_{i,\sigma} z_{j,\sigma} \sum_{k=1}^{N_{el}} \Phi^*_{i,\sigma}(k) \Phi_{j,\sigma}(k) + U \sum_i d^2_i + \sum_{i \neq j,\sigma\sigma'} V_{ij} \sum_{k,k'} \Phi^*_{i,\sigma}(k) \Phi_{i,\sigma}(k) \Phi^*_{j,\sigma'}(k') \Phi_{j,\sigma'}(k') \tag{2}$$

which has to be minimized with respect to the fermionic wavefunctions and bosonic fields within the orthonormality and completeness constraints (for further details of this approach see [15]).

Single-stripe calculation. – In the presence of LR interactions a single stripe will always result unstable with respect to isolated polarons by increasing the length of the stripe. Indeed the Coulomb energy per hole of a charged wall of length L increases as $\log L$ and it is not compensated by the coupling to a uniform distribution of background charges of opposite sign, as it is the case for a regular array of stripes. Nevertheless the analysis of the single-stripe case allows to illustrate the stabilization effect of a large U (within the Gutzwiller approach and with respect to the HF treatment) and to find out the most stable stripe configuration within each class of stripes.

It has been intensively discussed in Ref. [14] that for the half-filled wall to become a saddle-point for any effective one-particle description, it is necessary to quadruple the period along the stripe. In fact there exist several possibilities of performing this period quadrupling and in Fig. 1 we sketch the charge- and spin structures of the two types of half-filled vertical domain walls which have the lowest energy among the different realizations. We find that the stripe configurations investigated in Ref. [14] (cf. Figs. 8,9 therein) are always higher in energy than the structures shown in Fig. 1.

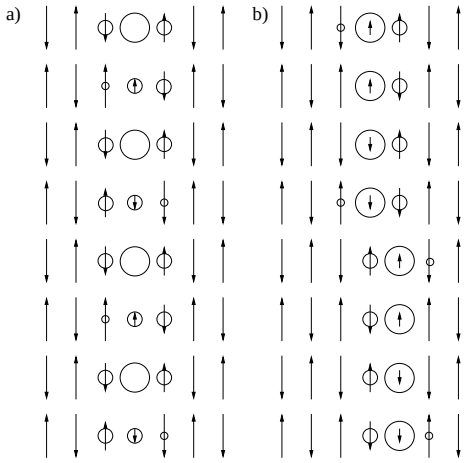

FIG. 1. Charge- and spin-density structure for the two half-filled vertical domain wall types described in the text. The diameter of the circles indicates the hole charge and the length of the spin arrows symbolizes the value of $\langle S_z \rangle$.

Fig. 1(a) is of the CDW type where the main charge modulation is with $q^c_\parallel = \pi$ along the wall whereas the spin varies with $q^s_\parallel = \pi/2$. We find that among the half-filled vertical walls this configuration is lowest in energy in the range $4t < U < 7.5t$. However, for strong on-site repulsion ($U > 7.5t$) the charge and spin realization with the lowest energy corresponds to the staggered structure indicated in Fig. 1(b) although the difference in energy to the CDW-type of Fig. 1(a) is rather small (the difference in energy per hole for $U = 10t$ is $\approx 5 * 10^{-3} t$).

For the single stripe solutions the size of the supercell is 9×8. Calculation of the diagonal structures for periodic boundary conditions without frustrating the background spin configuration in principle requires an 'uneven $\times$ uneven' lattice which does not allow for the investigation

of half-filled diagonal walls. For this reason and to avoid the comparison between different lattice sizes for different domain wall types we have choosen supercells with periodic boundaries for vertical stripes and with shifted periodic boundaries for diagonal stripes. In the 'shifted boundaries' the equivalent supercells in the vertical direction are horizontally shifted by one lattice spacing (cf. Fig. 4 in Ref. [15]). To avoid double counting in the Coulomb interaction energies, we cut off the LR forces at "half-minus-one" the size of the supercell.

The energy *per hole* of each configuration was calculated with respect to the reference state of a uniform AF lattice with one particle per site: $E(config) = (E(N_h) - E_{AF}(0))/N_h$ [17]. In particular the energy of an isolated spin-polaron is given by $E(polaron) = E(N_h = 1) - E_{AF}(0)$. To compare the stability of stripes on our finite-size system, we report the energy differences $E(config) - E(polaron)$.

The results are displayed in Fig. 2 as a function of the nearest neighbor value of the Coulomb repulsion $V_{n,n+1}$ for $U = 7t$ in Fig. 2(a) and for $U = 10t$ in Fig. 2(b). In case of half-filled vertical stripes the curves in Fig. 2(a) and 2(b) correspond to the structures in Fig. 1(a) and 1(b) respectively.

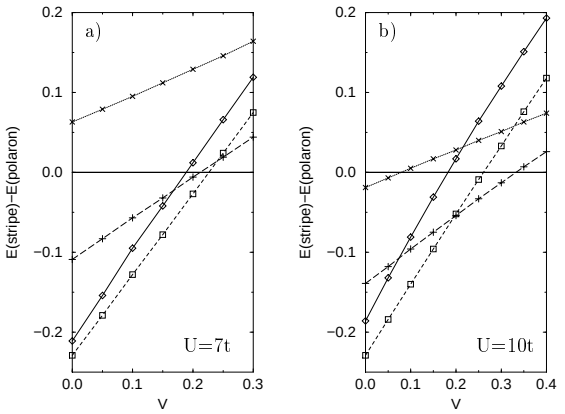

FIG. 2. Energy difference of various striped phases and the isolated polaron lattice $E(stripe) - E(polaron)$ as a function of the nearest neighbor contribution $V_{n,n+1}$ to the long-range potential. Solid line ($\diamond$): completely filled vertical stripe; long-dashed line (+): half-filled vertical stripe; short-dashed line ($\Box$): completely filled diagonal stripe; dotted line ($\times$): half-filled diagonal stripe. System size: 9×8; a) U=7t; b) U=10t.

Disregarding the eventual above-mentioned instability of the single stripes with respect to isolated polarons by increasing lenght, various features are worth noting. First of all, completely filled stripes increase more rapidly their energy (have a larger slope) than half-filled ones upon increasing the LR repulsion. Therefore LR forces favor half-filled stripes, which eventually become the most favorable wall textures.

However, the most relevant effect to be noticed here is the role of a large local repulsion U affecting the energies of the various textures. In particular a comparison between Fig. 2(a) and Fig. 2(b) shows that U strongly reduces the energy of the half-filled stripes with respect to the filled ones already at $V = 0$. By combining this reduction with the effects of LR forces on the stripes it follows that increasing U makes the half-filled vertical stripe the most stable among the wall solutions at smaller values of $V_{n,n+1}$.

Interstripe interaction and spin-polaron lattice. – To assess the actual ground state we now consider the interaction between stripes or between spin polarons. Indeed one cannot neglect the interstripe repulsion since, for example, in $La_{1.48}Nd_{0.4}Sr_{0.12}CuO_4$ the stripe separation is four times the Cu-Cu distance only. To incorporate the repulsion between stripes, we have calculated the energy of vertically oriented stripes on a 32×4 lattice. For a concentration of 1/8 this results in an array of 4 completely filled or 8 half-filled stripes. The energy of these arrays with respect to the polaronic Wigner lattice are depicted in Fig. 3 (the Wigner lattice now corresponds to 16 spin polarons with maximum distance).

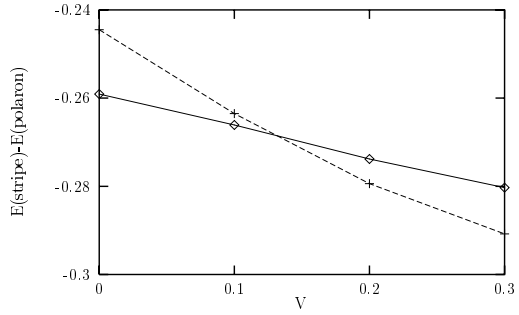

FIG. 3. Energy difference between vertically striped phases and the 'interacting' spin-polaron Wigner lattice as a function of the nearest neighbor contribution $V_{n,n+1}$ to the long-range potential (in units of t). Solid line ($\diamond$): completely filled vertical stripe; long-dashed line (+): half-filled vertical stripe. System size 32×4, U=10t.

In this case we obtain a crossover to half-filled vertical domain walls for $V \approx 0.12t$. It is interesting to observe that now the stripe solutions gain in energy upon switching on the LR part with respect to the polaron lattice. This enhances the parameter range of stability for the stripes, which no longer become unstable towards the decay into isolated polarons.

To assess the absolute stability of the half-filled vertical stripes, we should also compare their energy with the filled diagonal stripes, which, in the single-stripe analysis result to be more stable than the filled vertical stripes. However, filled diagonal stripes are strongly destabilized by the elongated shape of the 32×4 supercell so that we do not included their energy in Fig. 3. As an alternative to the direct calculations on the elongated cluster, to extract informations about diagonal stripe config-

urations, we analyzed a twodimensional regular array of charged wires with fixed global charge density. We have found that the electrostatic potential energy is lower for wires with higher linear charge density at a larger distance than for less charged wires more closely spaced. Therefore diagonal stripes, which at given planar density are closer by $\sqrt{2}$, but less densely charged by the same factor, are less favorable than the vertical stripes as far as the electrostatic Coulombic energy is concerned. On the other hand, our single-stripe investigation already demonstrated that a proper treatment of the strong local repulsion U opens the way to a stabilization of half-filled vertical stripes with respect to the filled diagonal stripes. From the above purely electrostatic analysis and from the results of Fig. 3 we can therefore safely conclude that half-filled vertical stripes are the ground-state configuration for $V \gtrsim 0.12t$ at large enough U.

To summarize, we have shown that a LR Coulomb interaction added to the 2D Hubbard model gives rise to half-filled vertically oriented domain walls when treated within an unrestricted Gutzwiller approach. This feature does not appear in semiclassical Hartree-Fock approximations where the effective attraction between spin-polarons is underestimated. Depending on the value of the on-site repulsion U, we expect the domain wall structure in the Nd-doped LaCuO system to be of the type shown in Fig. 1(a) and Fig. 1(b), respectively. Moreover, the here investigated competition between completely filled diagonal and half-filled vertical stripes can explain the different hole orderings in nickelates and in Nd cuprates even without invoking a relevant role of lattice interactions. Specifically, our findings suggest that nickelates could be characterized by a smaller $U \lesssim 7t$ and/or a smaller V accounting for their filled diagonal stripes. On the other hand, although the half-filled vertical stripes in the Nd-enriched LaSrCuO systems are to some extent likely fixed along the (1,0) direction by the underlying lattice structure, we showed here that, if large values of U and sizable values of V characterize these systems, then electronic correlations would also contribute to give rise to vertically half-filled stripes.

In general the filling and orientation of the stripes depend on the specificity of the electronic forces and structures and therefore inside the various oxide families different textures of the stripe phase may prevail.

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